

A Unitary Fermi Supersolid: The Larkin-Ovchinnikov Phase

Aurel Bulgac and Michael McNeil Forbes*

Department of Physics, University of Washington, Seattle, WA 98195-1560, USA

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We present strong theoretical evidence that a Larkin-Ovchinnikov (LOFF/FFLO) pairing phase is favoured over the homogeneous superfluid and normal phases in three-dimensional unitary Fermi systems. Using a Density Functional Theory (DFT) based on the latest quantum Monte-Carlo calculations and experimental results, we show that this phase is competitive over a large region of the phase diagram. The oscillations in the number densities and pairing field have a substantial amplitude, and a period some 3 to 10 times the average interparticle separation. Within the DFT, the transition to a normal polarized Fermi liquid at large polarizations is smooth, while the transition to a fully-paired superfluid is abrupt.

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The BCS mechanism for fermionic superfluidity is rooted in the notion of pairing: Can superfluidity survive in polarized systems with unequal numbers? This question remains largely unanswered, even though it is fundamental to many forms of matter, including superconductors, nuclear matter, and high density QCD. The prospect of observing exotic polarized superfluids has been revived in two-component cold-atoms gases with s -wave interactions, especially in the unitary limit where the scattering length diverges: $|a| \rightarrow \infty$. Here, the physics is universal, and inherently strongly coupled, depending solely on the densities. These systems are experimentally tenable (see Ref. [1] for a review), and exhibit a remarkable diversity of polarized phases.

Clogston and Chandrasekhar [2] noted that the normal phase competes with BCS superfluidity when the chemical potential difference between the species becomes comparable to the energy gap. Kohn and Luttinger [3], however, showed that interactions render Fermi surfaces unstable at sufficiently low temperatures, suggesting pairing of higher angular momenta. This effect is exponentially suppressed in weak coupling, but may be strong enough in unitary gases to support symbiotic p -wave superfluids [4]. Another proposal by Fulde and Ferrell (FF) [5], and Larkin and Ovchinnikov (LO) [6] – anisotropic/inhomogeneous polarized superfluids, widely referred to as LOFF or FFLO states – have also been vigorously sought (see [7] for reviews), but firm results have been sparse: Experimentally there have been claims of quasi-two-dimensional FFLO states in heavy-fermion superconductors [8], but no 3D realizations have been reported. Other proposals include deformed Fermi surfaces [9] and gapless (breached pair) superfluids [10].

We present here strong evidence that an inhomogeneous Larkin-Ovchinnikov (LO) state [6] may be realized in cold polarized unitary Fermi gases. Our approach is novel in several respects: 1) it is the first calculation to find a completely self-consistent LO solution in three dimensions; 2) the calculation is based on a Density Functional Theory (DFT) incorporating the best Monte-Carlo

calculations and measurements of the unitary Fermi gas; and 3) includes both pairing and self-energy correlations.

Previous calculations of LO states have not been fully self-consistent, often relying on approximate forms of spatial variations, or uncontrolled Ginzburg-Landau expansions (see e.g. Refs. [7, 11, 12]). Furthermore, self-consistent treatments are typically based on mean-field or Bogoliubov-de-Gennes (BdG) calculations, which do not properly account for many-body effects such as the Gorkov-Melik-Barkhudarov corrections [13] that lead to significant decreases in the pairing gap. Finally, most calculations account for only the pairing condensation energy, which is exponentially suppressed in weak-coupling, while the LO state has density variations that can significantly change the unsuppressed normal correlation energy (“Hartree” terms). Mean-field and BdG calculations neglect these crucial correlation contributions: Without them, LO states are not competitive at unitarity.

According to the theorems of Hohenberg and Kohn, a DFT exists for any system of fermions. At unitarity, the structure of the functional is strongly constrained by dimensional arguments, and thus its determination is greatly simplified. The remarkable accuracy of this approach for symmetric systems – as demonstrated in Ref. [14] – gives us the confidence to extend the approach to polarized systems. To model the polarized unitary Fermi gas, we use an asymmetric (ASLDA) generalization of the superfluid local density approximation (SLDA) employed in Ref. [14], expressed in terms of the following densities

$$\begin{aligned} n_a(\mathbf{r}) &= \sum_{E_n < 0} |u_n(\mathbf{r})|^2, & n_b(\mathbf{r}) &= \sum_{0 < E_n} |v_n(\mathbf{r})|^2, \\ \tau_a(\mathbf{r}) &= \sum_{E_n < 0} |\nabla u_n(\mathbf{r})|^2, & \tau_b(\mathbf{r}) &= \sum_{0 < E_n} |\nabla v_n(\mathbf{r})|^2, \\ \nu(\mathbf{r}) &= \frac{1}{2} \sum_{E_n} \text{sign}(E_n) u_n(\mathbf{r}) v_n^*(\mathbf{r}), \end{aligned} \quad (1)$$

where $u_n(\mathbf{r})$, $v_n(\mathbf{r})$, and E_n are the quasiparticle wavefunctions and energies [14]. We use the same functional form as Ref. [14], but allow the parameters to depend on

the local asymmetry $x(\mathbf{r}) = n_b(\mathbf{r})/n_a(\mathbf{r})$. The resulting ASLDA energy density $\mathcal{E}(\mathbf{r})$ has the form

$$\mathcal{E}(\mathbf{r}) = \frac{\hbar^2}{2m} \left[\alpha_a(\mathbf{r}) \tau_a(\mathbf{r}) + \alpha_b(\mathbf{r}) \tau_b(\mathbf{r}) \right] + g_{\text{eff}}(\mathbf{r}) |\nu(\mathbf{r})|^2 + \frac{3(3\pi^2)^{2/3} \hbar^2}{10m} \left[n_a(\mathbf{r}) + n_b(\mathbf{r}) \right]^{5/3} \beta[x(\mathbf{r})], \quad (2)$$

where $\alpha_a(\mathbf{r}) = \alpha[x(\mathbf{r})]$ and $\alpha_b(\mathbf{r}) = \alpha[1/x(\mathbf{r})]$ are the inverse effective masses in units of m^{-1} defined in terms of the single function $\alpha(x)$, $\beta(x) = \beta(1/x)$ parametrizes the normal interaction, and $(n_a + n_b)^{1/3}/\gamma = 1/g_{\text{eff}} + \Lambda$ defines the effective coupling g_{eff} that is regulated with the cutoff Λ as described in Refs. [14, 15]. The forms of $\alpha(x)$ and $\beta(x)$ are well constrained by Monte-Carlo data, as described below and in Ref. [15]. The equations for the quasiparticle wave-functions $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$ follow by minimizing the grand-canonical functional

$$\Omega = -\int d^3\mathbf{r} \mathcal{P}(\mathbf{r}) = \int d^3\mathbf{r} \left[\mathcal{E}(\mathbf{r}) - \mu_a n_a(\mathbf{r}) - \mu_b n_b(\mathbf{r}) \right],$$

where $\mu_{a,b}$ are the chemical potentials corresponding to the two fermion species, and $\mathcal{P}(\mathbf{r})$ is the local pressure.

We must now specify the forms of $\alpha(x)$ and $\beta(x)$. First we analyze the symmetric superfluid phase as described in Refs. [14, 15]. By matching the Monte-Carlo values [16, 17, 18, 19] for the parameters $\xi = \mathcal{E}_{SF}/\mathcal{E}_{FG} = 0.40(1)$, $\eta = \Delta/\varepsilon_F = 0.504(24)$, and the single quasiparticle excitation spectrum, we determine the inverse effective mass $\alpha(1) \approx 1.09(2)$, the constant $\gamma^{-1} = -0.091(8)$, and the implied energy of the symmetric normal phase $\xi_N = \mathcal{E}_N/\mathcal{E}_{FG} = \alpha(1) + \beta(1) = 0.57(2)$. In Ref. [14] it was erroneously stated that $\alpha(1)$ could be extracted from the values of ξ and η alone. A more careful analysis shows that the quasiparticle dispersion [17] must also be fit, resulting in the modified SLDA parameters presented here. The inverse masses $\alpha_{a,b}$ are also known for the fully-polarized gas. The majority species is unaffected, whereas the minority species has the effective “polaron” mass $m/m^* \approx 1.04(3)$ [20, 21], constraining the endpoints $\alpha(0) = 1$ and $\alpha(\infty) = 0.96(3)$. To determine the function $\beta(x)$, we consider the energy of the interacting normal state, setting $\Delta \equiv 0$. This has been well constrained by Monte-Carlo calculations [16, 20], and, along with the parametrization of $\alpha(x)$, a fit to this data uniquely specifies the function $\beta(x)$ (see Fig. 1).

In this paper, we consider only the simplest LO states, with spatial modulations in a single direction (z). Unlike the FF state [5], the LO state [6] does not break time-reversal invariance, and thus belongs to a different symmetry class, as was emphasized by Yoshida and Yip [11]. We do not consider FF states here as they are typically not competitive with the LO states. (FF states break time-reversal invariance, and require additional terms in (2) to restore Galilean invariance [14, 15].)

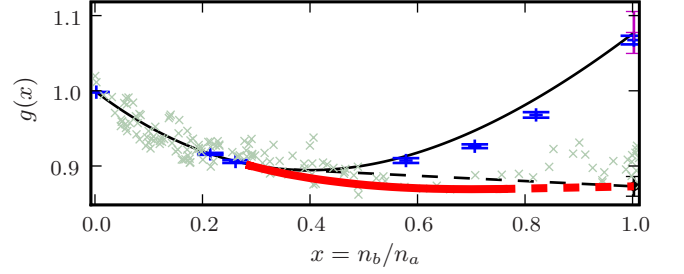


FIG. 1: (Color online) The dimensionless convex function $g(x)$ [22] that defines the energy density $\mathcal{E}(n_a, n_b) = \frac{3}{5} \frac{\hbar^2}{2m} (6\pi^2)^{2/3} [n_a g(x)]^{5/3}$. The points with error-bars (blue online) are the Monte-Carlo data from Refs. [20]. The fully-paired solution $g(1) = (2\xi)^{3/5}$ is indicated to the bottom right, and the recent MIT data [23] is shown (light \times) for comparison. The phase separation discussed in Refs. [20] is shown by the Maxwell construction (thin black dashed line) of the 1st-order transition $y = y_{N-SF}$ in Fig. 2. The LO state (thick red curve) has *lower energy* than all pure states and phase separations previously discussed. The Maxwell construction of the weakly 1st-order transition $y = y_{LO-SF}$ in Fig. 2 is shown by the thick dashed line (red).

The self-consistency equations are solved by discretizing the Hamiltonian along z with a discrete variable representation (DVR) basis [24] of period L , while integrating over the perpendicular momenta and the Bloch states. Our quasiparticle wave-functions thus satisfy the conditions $u_n(x, y, z + L) = e^{i\phi_n} u_n(x, y, z)$, $v_n(x, y, z + L) = e^{i\phi_n} v_n(x, y, z)$, and are plane waves in the (x, y) plane. We minimize the truncation error due to the finite DVR basis set by using a smoothed version of the hybrid strategy [25], summing discrete states with energies less than a cutoff E_c , while integrating over the remaining higher-energy semi-classical states.

We start by specifying chemical potentials μ_a and μ_b , and an ansatz for $\Delta(z) \propto \sin(2\pi z/L)$ containing a node at $z = 0$, and then use a Broyden iteration scheme [26] to find a self-consistent solution. The choice of basis and iteration preserve the node at $z = 0$, converging to either a self-consistent LO state, or degenerating to a homogeneous normal state with $\Delta(z) = 0$ everywhere.

The resulting self-consistent states depend on the external parameter L . To find the physical LO state, we vary L to find the spontaneously chosen length scale $L = L_{LO}$ that minimizes the potential Ω (maximizes the average pressure \mathcal{P}). The search is aided by the relationship $L \partial \mathcal{P} / \partial L = 2\mathcal{E} - 3\mathcal{P}$ between L , the average pressure, and the energy density [15], ensuring the unitary relationship $\mathcal{P} = \frac{2}{3}\mathcal{E}$ is satisfied by the physical state.

At unitarity, one may fully characterize all stable phases by the single parameter $y = \mu_b/\mu_a$ as described in Ref. [22]. We use the grand canonical ensemble, where only pure phases appear, and which properly accounts for the phase separation that occurs at 1st-order transi-

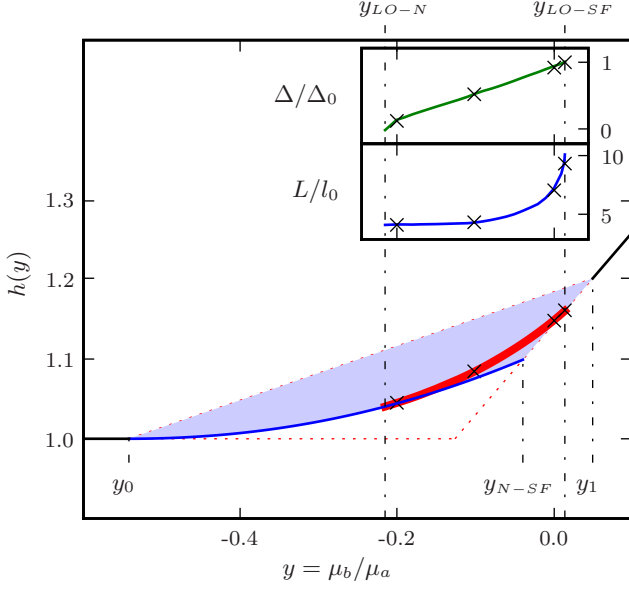


FIG. 2: (Color online) The dimensionless convex function $h(y)$ [22] that defines the average pressure $\mathcal{P}(\mu_a, \mu_b) = \frac{2}{5} \left(\frac{2m}{\hbar^2} \right)^{3/2} [\mu_a h(y)]^{5/2} / (6\pi^2)$ is constrained to the thin dotted triangular region [22]. The interacting normal state pressure [20] defining our ASLDA functional constrains this further (thin blue line), and displays a 1st-order transition at y_{N-SF} where normal and SF phases could coexist (Maxwell construction in Fig. 1). The LO state has an even higher pressure (thick red line), replacing much of this region, including the former y_{N-SF} transition. The y dependence of the amplitude of the pairing field $\Delta = \max\{|\Delta(z)|\}$ and the period L are shown inset. Sample profiles for the states marked \times are shown in Fig. 3. Units are fixed in terms of $\mu_- = (\mu_a - \mu_b)/2$ [28].

tions (kinks in $h(y)$, discontinuities in $h'(y)$: see Fig. 2). We start by describing the homogeneous and isotropic states supported in the ASLDA functional: For $y < y_0$ [22], the system is a fully-polarized non-interacting Fermi gas (N_a); between $y_0 < y < y_{N-SF}$ the highest pressure corresponds to a partially polarized two-component Fermi gas; and above $y_{N-SF} < y < 1$, the fully-paired superfluid (SF) has the highest pressure. The point y_{N-SF} , where the pressures of the partially polarized normal and fully-paired superfluid states are equal, is where the phase-separation discussed in Refs. [20] would occur. Here, the competition to LO from the normal and superfluid states is minimized, and the LO state is most likely to occur. For $y > 1$, the picture is reversed with the species $a \leftrightarrow b$ exchanged. Our ASLDA parametrization does not admit any stable homogeneous gapless superfluid (breached pair) states [10].

As shown in Fig. 2, we find competitive LO solutions for a large range of the parameter $y \in (y_{LO-N}, y_{LO-SF})$ with finite periods in the range $L_{LO-N} \leq L \leq L_{LO-SF}$. At y_{LO-N} , the transition appears to be second order, with

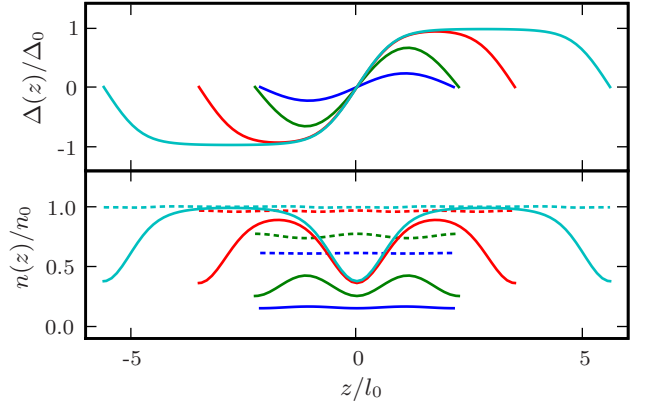


FIG. 3: (Color online) A single LO period showing the spatial dependence of the pairing field $\Delta(z)$ (top) and the number densities of the majority (dotted) and minority (solid) species (bottom) at the values of $y \in (y_{LO-N}, y_{LO-SF})$ marked by \times in Fig. 2. Units are fixed in terms of μ_- [28].

$\max\{|\Delta(z)|\} \rightarrow 0$ vanishing smoothly from the LO phase to the normal phase, while at y_{LO-SF} , the order parameter abruptly loses its spatial oscillations at a finite period L_{LO-SF} . Due to the presence of a node in $\Delta(z)$, the only possibility for a smooth transition here would be for the period to diverge $L_{LO-SF} \rightarrow \infty$, thus this transition appears to be weakly first order. The remaining normal states between $y_0 < y < y_{LO-N}$ would be susceptible to the Kohn-Luttinger instability, and are candidates for the symbiotic p -wave superfluids discussed in Refs. [4]. To study this possibility requires an extension of the ASLDA.

Fig. 3 shows the typical structure of a LO state. The pairing amplitude increases smoothly from zero at y_{LO-N} , where the profile is almost sinusoidal, to a critical value slightly less than Δ_0 at y_{LO-SF} , while the minority component exhibits large oscillations that break translation invariance, giving the LO state the crystalline properties of a quantum solid. The majority component exhibits much smaller oscillations because the larger local kinetic energy density suppresses gradients. These fluctuations induce large oscillation in the mean-field potentials (not shown), and have a significant impact on the normal correlation energy. For this reason, all the terms in the energy density functional are critical for a proper description of the LO phase.

If no other phases compete, one should observe that the LO-SF transition coincides with the termination point y_1 of the partially polarized phases PP_a [22]: $y_{LO-SF} = y_1$. A more complicated crystalline LO state with modulations in all three directions may further increase the average pressure, making $y_1 > y_{LO-SF}$. Current errors of the current Monte-Carlo calculations and experiments do not allow us to distinguish between these two cases. These results are summarized in Fig. 2, where it can be seen that these periodic LO solutions occupy a substantial

portion of the phase diagram, and lead to a significant increase in the average pressure. The Legendre transformed results have been included in Fig. 1 to facilitate comparisons with the Monte-Carlo data [20] and recent experiments [23].

In conclusion, we have shown that the ASLDA provides a valuable tool for quantitatively evaluating inhomogeneous phases. By incorporating the latest non-perturbative data about unitary Fermi gases, we have presented strong evidence that a new form of matter, such as a crystalline LO phase, is waiting to be found in the partially polarized regime of cold unitary Fermi gases. This would be the first example of a Fermi supersolid at unitarity, and with the large pairing gap, there is a good chance of successfully studying this state with cold atoms. In the experiments to date, the shells where LO phases may exist are too thin to allow for a complete LO period L . However, traps can be adjusted so that the LO phase will occupy a larger spatial region, allowing for several LOFF oscillations to occur. Unlike LO in weak coupling, the amplitude of the density fluctuations in the minority component is large and comparable to that of vortices [27] in unitary gases. This will provide the most direct signature of unitary supersolid matter, and an clean way to study the LOFF phase.

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* E-mail: mforbes@alum.mit.edu

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